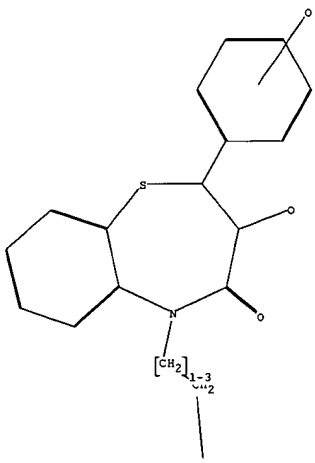
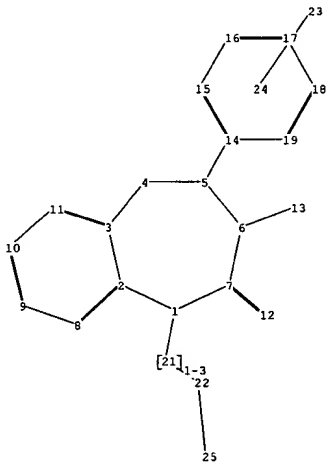
C:\STN4tmp\QUERIES\09456429_4.str

Update 10/5/05





Searched all (hetero compounds)

chain nodes :
12 13 21 22 23 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 14 15 16 17 18 19
chain bonds :
1-21 5-14 6-13 7-12 21-22 22-25
ring bonds :
1-2 1-7 2-3 2-8 3-4 3-11 4-5 5-6 6-7 8-9 9-10 10-11 14-15 14-19 15-16
16-17 17-18 18-19
exact/norm bonds :
1-2 1-7 6-13 7-12
exact bonds :
1-21 3-4 4-5 5-6 5-14 6-7 21-22 22-25
normalized bonds :
2-3 2-8 3-11 8-9 9-10 10-11 14-15 14-19 15-16 16-17 17-18 18-19
isolated ring systems :
containing 1 : 14 :

Some 103 type art

ie US 5378648
& US 5462936

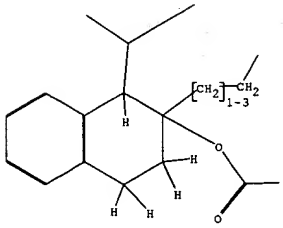
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS

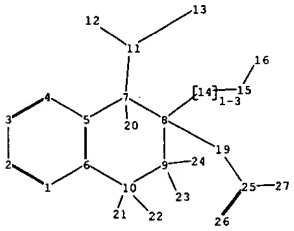
C:\STN4tmp\QUERIES\09456429_5.str

update 10/5

searched
and
for ligand (i)

NO ART



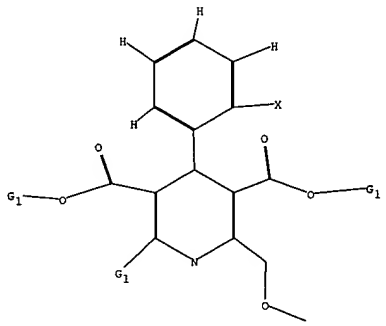


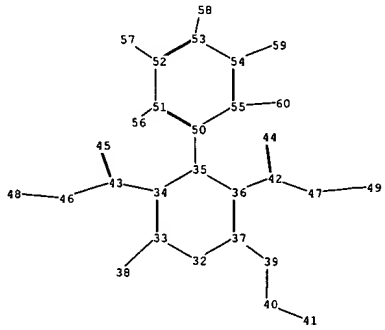
chain nodes :
11 12 13 14 15 16 19 20 21 22 23 24 25 26 27
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
7-11 7-20 8-14 8-19 9-23 9-24 10-21 10-22 11-12 11-13 14-15 15-16 19-25
25-26 25-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
5-7 6-10 7-8 8-9 8-19 9-10 19-25 25-26
exact bonds :
7-11 7-20 8-14 9-23 9-24 10-21 10-22 11-12 11-13 14-15 15-16 25-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

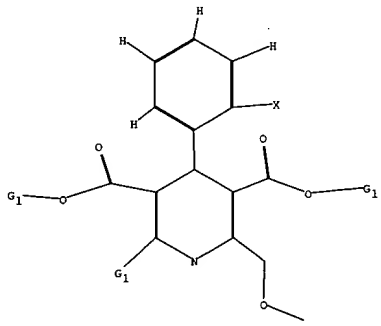
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS

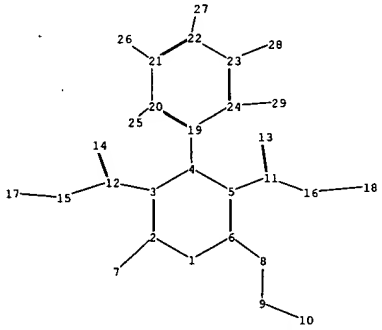
C:\STN4tmp\QUERIES\09456429_7.str

Update ID 5/05









only searched "trans dimers of ligand (ii)

102 art!

chain nodes :
7 8 9 10 11 12 13 14 15 16 17 18 25 26 27 28 29 38 39 40 41 42 43
44 45 46 47 48 49 56 57 58 59 60
ring nodes :
1 2 3 4 5 6 19 20 21 22 23 24 32 33 34 35 36 37 50 51 52 53 54 55
chain bonds :
2-7 3-12 4-19 5-11 6-8 8-9 9-10 11-13 11-16 12-14 12-15 15-17 16-18 20-25
21-26 22-27 23-28 24-29 33-38 34-43 35-50 36-42 37-39 39-40 40-41 42-44 42-47
43-45 43-46 46-48 47-49 51-56 52-57 53-58 54-59 55-60
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 19-20 19-24 20-21 21-22 22-23 23-24 32-33 32-37
33-34 34-35 35-36 36-37 50-51 50-55 51-52 52-53 53-54 54-55
exact/norm bonds :
1-2 1-6 2-3 2-7 3-4 4-5 5-6 8-9 9-10 11-13 11-16 12-14 12-15 15-17 16-18
32-33 32-37 33-34 33-38 34-35 35-36 36-37 39-40 40-41 42-44 42-47 43-45 43-46
46-48 47-49
exact bonds :
3-12 4-19 5-11 6-8 20-25 21-26 22-27 23-28 24-29 34-43 35-50 36-42 37-39
51-56 52-57 53-58 54-59 55-60
normalized bonds :
19-20 19-24 20-21 21-22 22-23 23-24 50-51 50-55 51-52 52-53 53-54 54-55

G1:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:CLASS 39:CLASS
40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS
49:CLASS 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 57:CLASS
58:CLASS 59:CLASS 60:CLASS